

# 17beta-Acetoxy-10-isoandrost-4-en-3-one

<b>Other names:</b>	Methyl 3-keto-4-etiocholenate 4-Androstene-17-carboxylic acid, 3-oxo-, methyl ester Androst-4-ene-17-carboxylic acid, 3-oxo-, methyl ester, (17«beta»)- Methyl 3-oxo-4-androstene-17beta-carboxylate Methyl-3-oxoandrost-4-ene-17B-carboxylate
<b>Inchi:</b>	InChI=1S/C21H30O3/c1-20-10-8-14(22)12-13(20)4-5-15-16-6-7-18(19(23)24-3)21(16,2)
<b>InchiKey:</b>	XWFWMYFLNHTEBF-NLPWGACESA-N
<b>Formula:</b>	C21H30O3
<b>SMILES:</b>	COC(=O)C1CCC2C3CCC4=CC(=O)CCC4(C)C3CCC12C
<b>Mol. weight [g/mol]:</b>	330.46
<b>CAS:</b>	2681-55-2

## Physical Properties

Property code	Value	Unit	Source
gf	-54.14	kJ/mol	Joback Method
hf	-562.76	kJ/mol	Joback Method
hfus	24.86	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.307		Crippen Method
mcvol	268.020	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	2730.00		NIST Webbook
tb	867.58	K	Joback Method
tc	1115.31	K	Joback Method
tf	573.57	K	Joback Method
vc	1.010	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.49	J/molxK	867.58	Joback Method
cpg	971.99	J/molxK	908.87	Joback Method
cpg	998.46	J/molxK	950.16	Joback Method

cpg	1025.25	J/mol×K	991.45	Joback Method
cpg	1052.70	J/mol×K	1032.74	Joback Method
cpg	1081.18	J/mol×K	1074.03	Joback Method
cpg	1111.01	J/mol×K	1115.31	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2681552&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2681552&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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